1. Calculate fingerprints

- 1011011...
- 1100010...
- 1010001...
- 1110110...
- 1011001...
- 1011111...
- 0100010...
- 1001111...
- 1010000...

2. Tanimoto similarity matrix

threshold = .7

	.3	.7	.4	.7	.9	.2	.5	.7
	.2	.8	.4	.6	.9	.7	.7	
	.4	.9	.7	.2	.6	.9		
	.5	.6	.9	.7	.6			
	.7	.3	.7	.8				
	.4	.9	.6					
	.5	.2						
	.7							

⇒ sort molecules by #neighbors (molecules with similarity ≥ .7)

	#neighbors
	4
	4
	4
	3
	5
	4
	2
	5
	5

sort ⇒

	#neighbors
	5
	5
	5
	4
	4
	4
	4
	3
	2

3. Clustering

Flag cluster members, start from top of the list:

1. Iteration: molecule

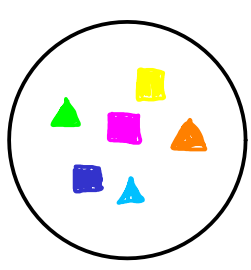
Neighbors:

	.3	.7	.4	**.7**	.9	.2	.5	.7
	.2	.8	.4	.6	.9	.7	.7	
	.4	**.9**	.7	.2	.6	.9		
	.5	.6	.9	.7	.6			
	.7	.3	**.7**	**.8**				
	.4	.9	.6					
	.5	.2						
	.7							

Flag neighbors (and centroid):

	.3	.7	.4	**.7**	.9	.2	.5	.7
	.2	.8	.4	.6	.9	.7	.7	
	.4	**.9**	.7	.2	.6	.9		
	.5	.6	.9	.7	.6			
	.7	.3	**.7**	**.8**				
	.4	.9	.6					
	.5	.2						
	.7							

Build new cluster:



2. Iteration: molecule

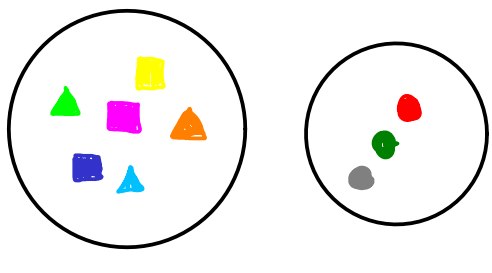
Neighbors:

	.3	.7	.4	.7	.9	.2	.5	.7
	.2	**.8**	.4	.6	**.9**	.7	.7	
	.4	.9	.7	.2	.6	.9		
	.5	.6	.9	.7	.6			
	.7	.3	.7	.8				
	.4	.9	.6					
	.5	.2						
	.7							

Flag neighbors (and centroid):

	.3	.7	.4	.7	.9	.2	.5	.7
	.2	**.8**	.4	.6	**.9**	.7	.7	
	.4	.9	.7	.2	.6	.9		
	.5	.6	.9	.7	.6			
	.7	.3	.7	.8				
	.4	.9	.6					
	.5	.2						
	.7							

Build new cluster:



3. Iteration → Termination, each molecule is part of a cluster.